

Pentadecane
629-62-9 | DTXSID6027268

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 7.24

Global applicability domain: Inside

Local applicability domain index: 9.65e-01

Confidence level: 5.90e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Hexachlorobenzene</div> <div>Measured: 7.38</div> <div>Predicted: 7.24</div>	<div>Image not found</div> <div>Lindane</div> <div>Measured: 8.30</div> <div>Predicted: 7.24</div>	<div>Image not found</div> <div>alpha-1,2,3,4,5,6-Hexachlorocyclohexane</div> <div>Measured: 8.30</div> <div>Predicted: 7.24</div>
<div>Image not found</div> <div>beta-Hexachlorocyclohexane</div> <div>Measured: 8.30</div> <div>Predicted: 7.24</div>	<div>Image not found</div> <div>delta-Hexachlorocyclohexane</div> <div>Measured: 8.30</div> <div>Predicted: 7.24</div>	<div>Image not found</div> <div>3-Chlorobiphenyl</div> <div>Measured: 6.82</div> <div>Predicted: 7.19</div>
<div>Image not found</div> <div>4-Chlorobiphenyl</div> <div>Measured: 6.80</div> <div>Predicted: 7.19</div>	<div>Image not found</div> <div>Fluorene</div> <div>Measured: 6.79</div> <div>Predicted: 7.07</div>	

